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COMPUTATIONAL FLUID DYNAMICS
AND AEROTHERMODYNAMICS

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Semiannual Progress Report
January 1987 - June 1987

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TAMRF Report No. 5671-87-01
July 1987

TEXAS A&M UNIVERSITY

Leland A. Carlson
Professor of Aerospace Engineering
Texas A&M University
College Station, TX. 77843-3141

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TEXAS AEROSPACE ENGINEERING EXPERIMENT STATION

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TAMRF Project RF 5671

Leland A. Carlson
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COMPUTATIONAL FLUID DYNAMICS AND AEROTHERMODYNAMICS
(Development of Nonequilibrium Models Applicable to AOTV/AFE and
Superorbital Flight Regimes)

I. Introduction

This report covers the period from January 7, 1987 thru June 30, 1987. It will briefly describe and summarize the current status of the project, the research efforts during the last six months, and projected future efforts. In addition, copies of viewgraphs recently used during a briefing to Johnson Space Center (JSC) personnel are included as an appendix.

II. Status and Personnel

Officially, the present project was awarded on January 7, 1987. However, final paperwork was not completed until the middle of February; and by this time personnel assignments for spring semester had already been decided. Consequently, no graduate students were assigned to this project until April 1, 1987. Due to this delayed start on the project, it may be necessary to request a no-cost extension to the project sometime in the next few months.

At the present time, the staff associated with the project are:

Leland A. Carlson -- Principal Investigator

Approximately 1/4 time

Glenn Bobskill -- Graduate Research Assistant

April - May, Half time

June to present, Full time

Thomas Gally -- Graduate Research Assistant

June to present, Half time

Robert Greendyke -- Graduate Research Assistant

June to present, Full time

The research work associated with this project will form the basis for the Masters thesis work of Mr. Bobskill and Mr. Greendyke. Mr. Gally received his Masters degree in May 1987 and is currently working on his doctoral degree. His current research efforts are split between this project and one involving transonic wing design and analysis.

III. Research Progress

At the present time the efforts on this project are organized into two areas. The first involves Tom Gally and Dr. Carlson and is directed towards the development of an approximate stagnation point solution. The second is directed towards approximate flowfield studies which can be used to develop and investigate shock jump, electron temperature, radiation, vibration-dissociation coupling, and chemistry models. The individuals associated with this second portion of the project are Dr. Carlson, Bob Greendyke, and Glenn Bobskill.

Approximate Stagnation Point Solution Studies

The objective of this effort is to develop a rapid and "accurate" approximate stagnation point solution which can be used for parameteric and/or design studies and which includes approximately the effects of chemical and thermal nonequilibrium, thermal conduction, radiative gasdynamic coupling, and convective and radiative heat transfer. Since this model is currently under development and undergoing daily revision, presentation of details will be delayed until later reports. However, a general outline of the approach is presented in the appendix. At the present time, computer solutions complete with graphics are being obtained in an interactive fashion; and the entire approach appears promising.

An example of the type of results which can be obtained with the present approximate solution is shown on Figure 1. This case is for a freestream velocity of 16 km/sec, an altitude of approximately 63.5 km., and a shock detachment distance of 5.88 cm. As can be seen, the flow rapidly equilibrates behind the shock wave and is in chemical equilibrium over most of the shock layer. Also, the flow exhibits some radiative cooling and coupling as evidenced by the steady decrease in temperature and degree of ionization in the central equilibrium part of the shock layer.

Now, normally one would expect that radiative heating from the transparent portion of the spectrum would correlate with the freestream parameter $0.5 * (\text{Freestream Density}) * (\text{Freestream Velocity Cubed})$, which is

a measure of the kinetic energy flux or power per unit area in the freestream, and scale with the shock detachment distance. Interestingly, this case, under that logic, corresponds closely to the condition of peak heating observed in the FIRE II flight experiment even though that case was at about 10.48 km/sec and 53.77 km. The present solution does contain an approximation for the heating from the visible portion of the spectrum, which is essentially transparent; and when this value is adjusted to account for differences in shock stand-off distance, the result is about 350 watts/sq.cm. While the project has not yet obtained the actual FIRE numerical data, graphical plots of the measurements indicate that stagnation radiative heating values of 350 to 400 watts/sq.cm. were measured from the visible wavelength regions at the time of peak heating.

A result obtained from the current approximate method which corresponds more closely to a FIRE II trajectory point is shown on Figure 2. This result is in reasonable agreement with detailed computations recently presented by Bird (Reference 1) and obtained using the direct simulation Monte Carlo method. Again, the flow behind the shock front equilibrates relatively quickly and most of the flowfield is in chemical equilibrium. However, due to the lower freestream velocity, the degree of ionization is relatively low and there is very little radiative gasdynamic coupling.

As mentioned previously, the present method contains a highly approximate method of estimating the stagnation point heating due to radiative transfer from the visible region. In addition, a version of

the code is being developed which uses the resultant flowfield solution to compute a more accurate estimate of radiative heating. The latter approach uses a five step radiation model which includes emission and absorption from the vacuum ultraviolet (VUV) continuum and lines, visible continuum, and infrared (IR) lines. Figure 3 compares the present predictions with data from the FIRE II experiment. The measurements from FIRE II were only in the visible plus IR spectrum and only those results are shown. The present results are plotted over a horizontal band since the present trajectory point did not match exactly a FIRE II point. Thus, one end of the spread corresponds to a match in freestream velocity while the other corresponds to a match of altitude. Interestingly, the present results "surround" the experimental data.

However, in this investigators opinion, this good agreement should not be viewed as verification of the method but rather as an indication that it is relatively easy to match the FIRE data in the plotted wavelength region. Phrased differently, the radiative heat flux in the visible plus IR is not a sensitive indicator of the accuracy of a flowfield calculation or model.

Nevertheless, it is believed that the present five-step radiative heat transfer results are interesting. These results, which should be viewed as very preliminary, are as follows:

Wavelength (Angstroms)	Type	Heat Transfer (Watts/sq.cm.)
620-1100	VUV Continuum	0.035
1100-1300	VUV Continuum	51.89
1300-1570	VUV Lines	1219.
1570-7870	Visible Continuum	18.08
7870-9552	IR Lines	108.5

First, it should be noticed that in the visible plus IR region, most of the heating is from IR lines. This trend is in accord with shock tube data and calculations of other investigators. However, the most surprising feature, is the strong contribution from the VUV and in particular from VUV lines. While, the contribution from this region will depend strongly upon shock detachment distance (i.e. optical path length) and the degree of nonequilibrium, these results indicate that VUV radiation and not the visible may dominate. While this possibility has been ignored by many investigators (assuming that the VUV will all be absorbed and not reach the body), it is in agreement with the recent calculations of Bird and is implied in the comparison between the visible plus IR and total heating measured on FIRE II.

Considering the uncertainty of these results and the lack of shock tube data in this wavelength regime, consideration probably should be given to instrumenting the AFE to either measure heating from the VUV or to provide measurements from which it can be deduced.

During the next portion of the project, it is planned to continue development of the approximate stagnation point model. Tentatively, the following tasks will be conducted:

(1) Incorporate methods for accurately computing radiative heat transfer using a five step absorption coefficient model. These techniques will include the effects due to chemical and thermal nonequilibrium.

(2) Develop and include in the method appropriate techniques for computing the convective heat transfer to the stagnation point.

(3) Improve the chemistry correlations used in the method.

(4) Automate the method so that it is easy to use and suitable for parametric type studies.

(5) Consider and if possible include slip boundary conditions so as to extend the region of validity of the model.

(6) Use the model to perform parametric type studies and compare results to experimental and flight data.

Approximate Flowfield Solution Studies

The primary objective of this portion of the program is to develop and study a variety of models and approximate models for various physical phenomena associated with the flowfield. In order to develop such models, delineate their applicability, and determine the consequences of their usage, it is essential to have a rapid flowfield solver. After considerable investigation, it was decided to use for the flow solver a chemical and thermal nonequilibrium Maslen type of inverse

solver due to Grose (Reference 2). In this method, a shock shape is assumed and the flowfield and body shape are determined as part of the solution.

While a Maslen model utilizes many assumptions, experience by this and other investigators has shown that such models yield very good engineering type of results. In addition, this model, which is based on the Euler equations, has several distinct advantages to the present project. First, it is computationally very fast. Second, it can be utilized to compute the solutions along only a few selected streamlines for those situations in which an entire flowfield solutions is not needed. This aspect is very important currently since many studies will be needed to determine the effects etc. of using various approximate models. Finally, the selected Maslen approach should be able to model AOTV/AFE type of vehicles reasonably well since they are basically blunt sphere-cones.

Currently, the model has been coded and test runs have been conducted. These test cases have included chemical nonequilibrium (seven species and six reactions) as well as vibrational nonequilibrium, and some typical results are included in the Appendix. It is planned to use this flow solver to study shock jump, electron temperature, radiation, vibration-dissociation coupling, and reaction chemistry models.

One of the primary problems in solving chemical nonequilibrium blunt body flows with the Euler and/or Navier Stokes equations is the

disparate time scales between various phenomena. Typically, some of the chemical reactions have characteristic times much shorter than others and much shorter than the flow characteristic time. These differences make the resultant equations stiff, which often leads to stability problems and long computing times. However, from a physical standpoint, chemical reactions in air often proceed in steps. For example, oxygen dissociation occurs much more rapidly than nitrogen dissociation, and both occur faster than ionization. Thus, in various flight regimes it might be possible to essentially uncouple the processes by assuming that one or more of them is complete in the "shock front" and incorporating the effect into the shock jump conditions.

Consequently, work is currently in progress under this portion of the project to develop several shock jump approximations, incorporate them into the flowfield solver, and study their applicability, subsequent effects on the flowfield, and the computational effort (or savings) involved. Currently three types of shock jump conditions, in addition to the default condition of frozen mass fractions, are being developed. The first, under the assumption that conditions are such that oxygen dissociation occurs essentially immediately behind the front, will determine post shock conditions assuming that O_2 and O are in equilibrium with each other and that N_2 and all other species concentrations are frozen. It is believed that this approximation will be valid over the blunt body portion of much of the AOTV flight regime.

The second one is applicable only to pure N_2 and assumes that nitrogen dissociation occurs rapidly and that N_2 and N are in

equilibrium immediately behind the front. While not directly applicable to ATOV atmospheric flight, the use and study of this approximation will enable some rapid studies of superorbital velocity flight and should give insight into a variety of phenomena which are dominated or strongly influenced by ionization and nitrogen atoms. At speeds above 10 km/sec nitrogen atoms and ions are the primary species affecting radiative phenomena.

Finally, a shock jump approximation is being developed which assumes that both nitrogen and oxygen dissociation are essentially complete immediately behind the shock front and that N_2 and O_2 are in equilibrium with N and O. Again the validity and applicability of this approximation will be investigated.

Another area which must be modeled appropriately in order to accurately predict ATOV/superorbital flowfields is the electron temperature, which is the temperature which controls radiative emission and absorption. At velocities above 10 km/sec there are sufficient number of free electrons that theoretically the electron temperature should be determined by solving an electron energy equation. However, the inclusion of this highly coupled equation into the problem greatly increases the computational time required for solution. Consequently, an investigation and evaluation of various methods of approximating the electron temperature for this flight regime is being conducted..

On the other hand, for velocities below approximately 10 km/sec, it is generally accepted that the electron temperature is closely coupled

to the nitrogen vibrational temperature; and some researchers have suggested approximating the electron temperature by setting it equal to the nitrogen vibrational temperature. While this approach is quite good over the latter portion of the chemical relaxation zone behind the shock wave, previous experimental and theoretical studies by this author indicate that the peak electron temperature may be significantly lower than the peak nitrogen vibrational temperature and that the time of the peak may be later. These differences could be important in computing the resultant radiative emission. Consequently, various electron temperature models are being studied and will be incorporated into the flowfield program and evaluated.

In conjunction with the evaluation of electron temperature models, various radiation models are also being studied. Since this effort has just been initiated, details are not yet available. However, for temperatures above 8000 to 10000 K, it appears that step models based upon nitrogen atoms and ions will be adequate. However, such models might possibly be simplified, and this possibility will be investigated.

At lower velocities and/or temperatures molecular band radiation becomes important and current project studies have not definitely determined whether or not step models can be used. The work in this area will, of course, continue.

By far one of the most important areas being studied currently under the project is vibration dissociation coupling models. Vibration dissociation coupling strongly influences species concentration

variations, vibrational temperatures, and hence electron temperatures and radiative emission-absorption. Currently, the flowfield program has a coupled vibration dissociation (CVD) model; and this approximation is being modified to a coupled vibration dissociation vibration (CVDV) model. Eventually, it is planned to include in the program the option of using either of these two models along with the CVDV preferential model and the more recently proposed Park model (Reference 3). In addition, present project studies indicate that the choice of vibrational relaxation data and correlations can have a significant effect on results. Consequently, in the next period the similarities, differences, and consequences of using each of these models along with various relaxation data will be investigated for the AOTV regime.

In conjunction with vibration dissociation coupling efforts work has also started on investigating the effects of various reaction chemistry models. It is planned not only to perform parametric studies of various rates but also to determine the effect on the flowfield and heat transfer of various proposed reaction rate temperature dependence models. While historically reaction rates have used heavy particle translational temperatures, several investigators have proposed for various reactions using electron temperatures, vibrational temperatures, or combinations of various temperatures. Current studies indicate that these various choices can affect rates and the extent of nonequilibrium by orders of magnitude. Thus, work is in progress to modify the flow code to allow various temperature options. After this work is completed, studies will be conducted to determine the effect of various

temperature dependence models. It should be noted that for these studies the fact that the inverse flow code can be used to compute only a few streamlines will result in significant time savings.

IV. Future Efforts

As indicated above and based upon discussions during a recent present to NASA personnel, work during the next project period will continue the development of the various approximate codes. During the next reporting period these will be used as follows:

- (1) To perform parametric studies of shock jump, electron temperature, and radiation models.
- (2) To perform parametric studies of vibration dissociation chemistry coupling and reaction chemistry models.
- (3) For the evaluation of various approximate models.
- (4) For the evaluation of various approximations associated with stagnation point solutions and to perform parametric studies of the influence of various parameters on stagnation point heating.

Finally, it should be noted that the present effort is directed not only towards the AFE/AOTV velocity regime but also towards velocities above 10 km/sec. There are essentially two reasons for considering the higher velocities. First, investigation of superorbital phenomena and the development of engineering models for that regime will be of value for future lunar and Mars missions. Second, the entry velocity of 10 km/sec for the AOTV should be viewed only as a "maximum cruise" point.

As for any aerospace vehicle, the actual flight envelope used to determine the vehicle design must, in order to account for emergencies and various mission options, encompass a larger velocity and altitude range. Thus, those portions of the current studies which are directed at velocities above 10 km/sec are from an engineering standpoint also applicable to an AFE/AOTV type of vehicle.

V. References

1. Bird., G. A., "Nonequilibrium Radiation During Re-Entry at 10 km/s," AIAA Paper No. 87-1543, June 1987.
2. Grose, W. L., "A Thin-Shock Layer Solution for Nonquilibrium, Inviscid Hypersonic Flows in Earth, Martian, and Venusian Atmospheres", NASA TN-D-6529, December 1971.
3. Park, C., "Assessment of Two-Temperature Kinetic Model for Ionizing Air," AIAA Paper 87-1574, June 1987.

GRANT MONITOR

The NASA Technical Monitor for this project is Dr. Winston Goodrich, Mail Code ED3, NASA Johnson Space Center, Houston, Texas 77058.

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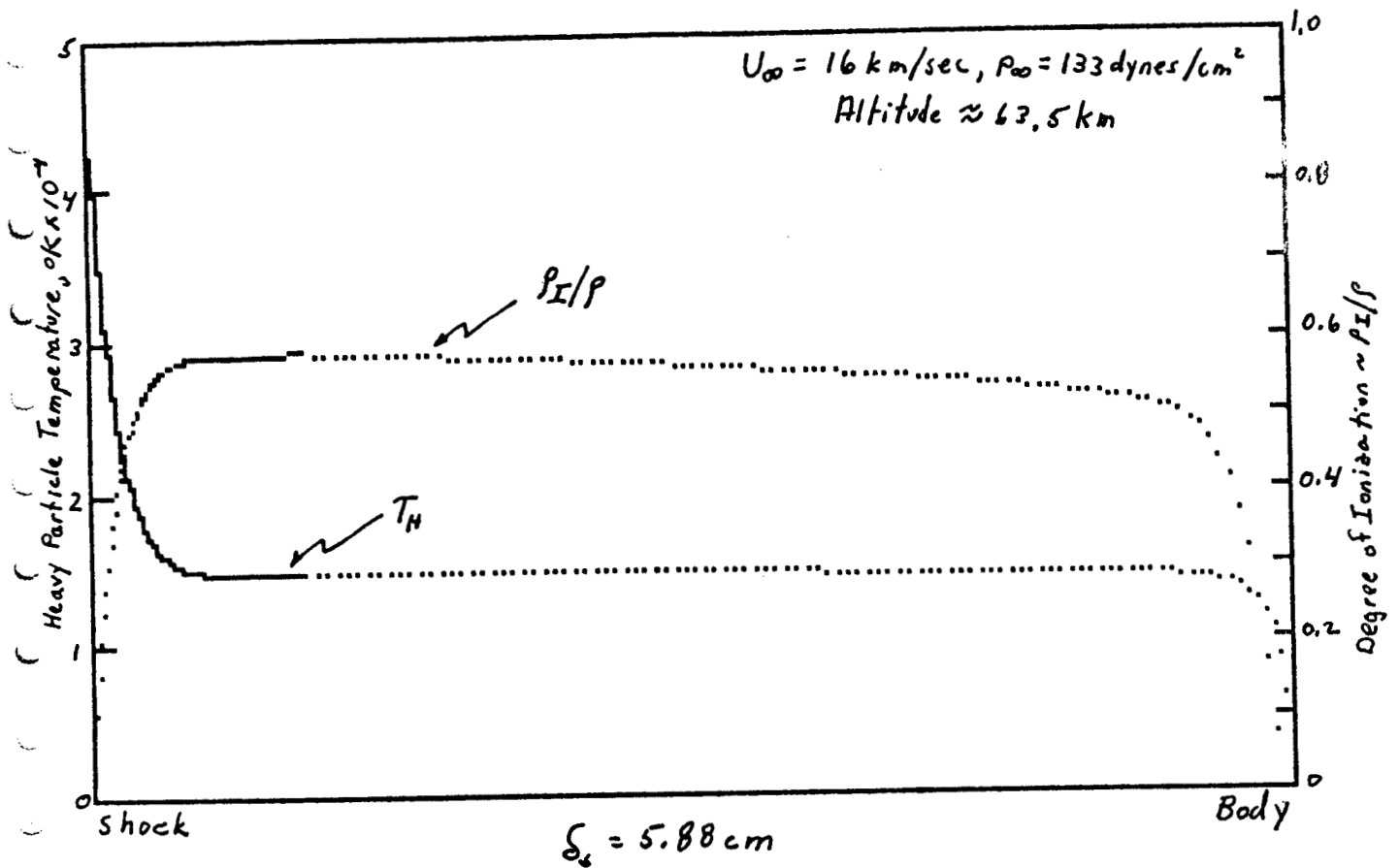


Figure 1-- Example of Approximate Stagnation Region Solution

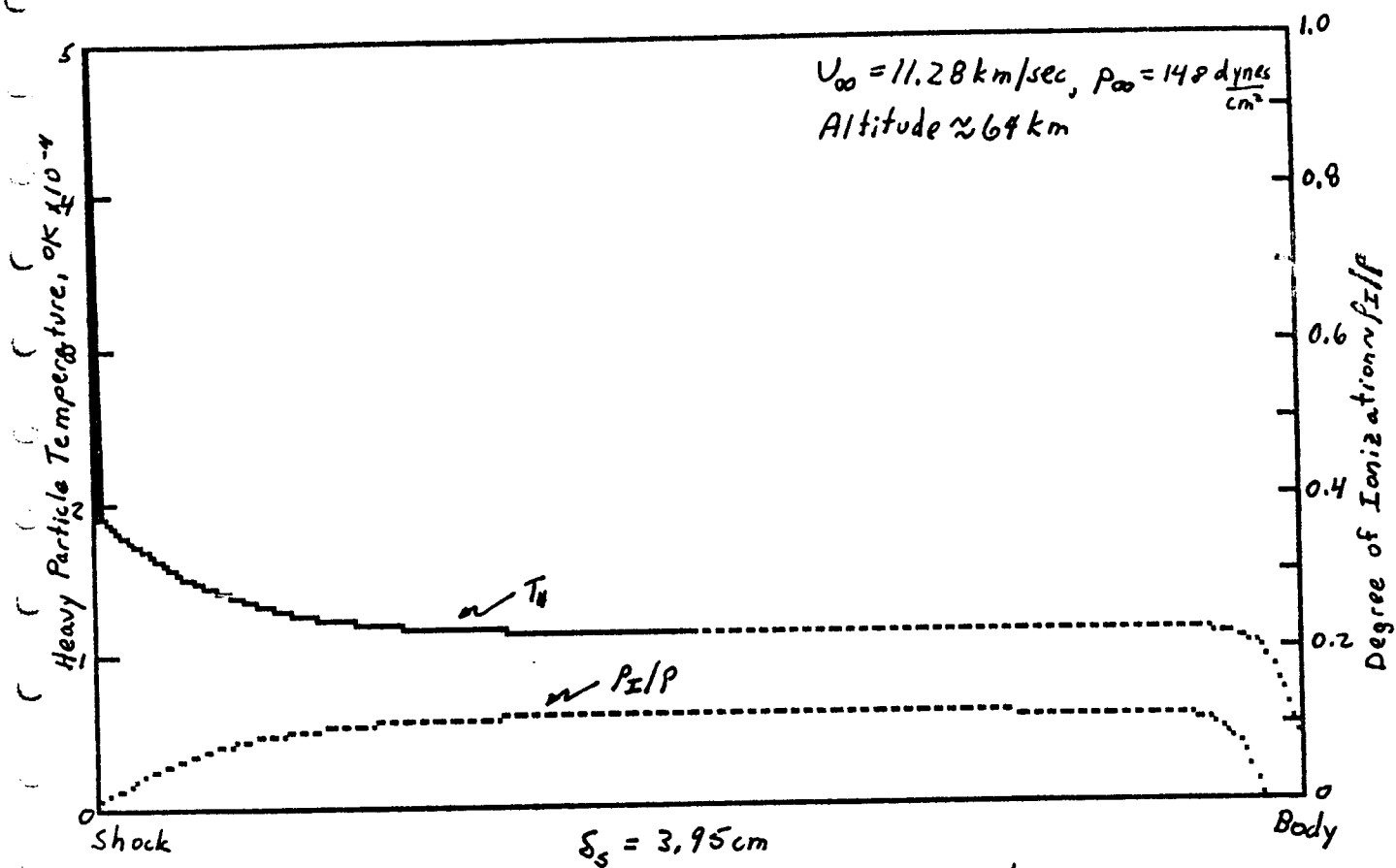


Figure 2 -- Approximate Fire II solution For Stagnation Region

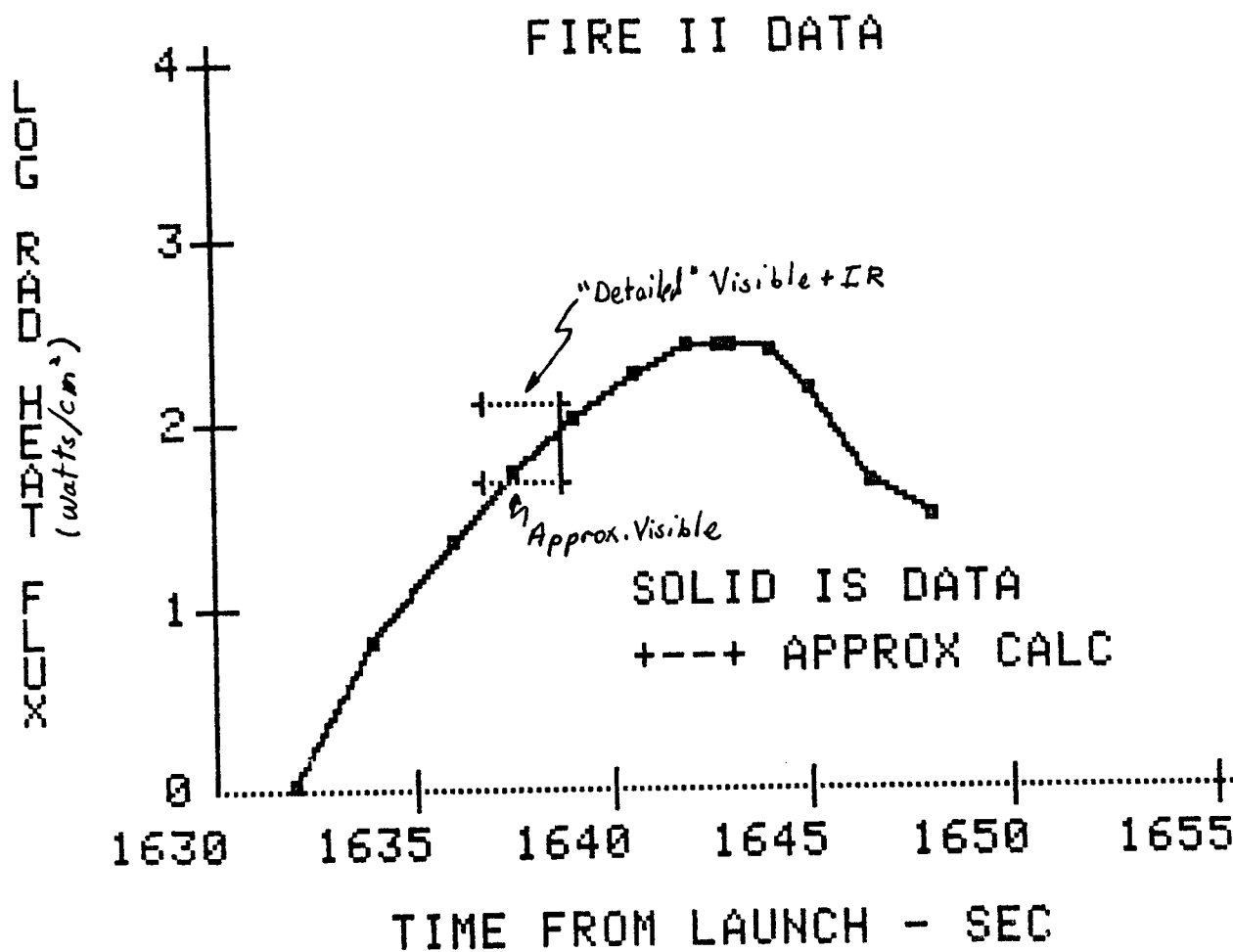


Figure 3-- Comparisons of Present Estimates with Data

APPENDIX

COMPUTATIONAL FLUID
DYNAMICS AND
AEROTHERMODYNAMICS

(Nonequilibrium Models Applicable to AOTV/AFE
Flight Regimes)

PROJECT STATUS

Effective Start Date: 1 April 87

TWO PARTS

PART I:

Approximate Stagnation Point Solution
(Gally and Carlson)

PART II:

Approximate Flowfield Solution Studies

- (a) Shock, Te, and Radiation
Approximations
(Greendyke and Carlson)
- (b) Vib.-Temp. Coupling Models and
Effect on Chemistry
(Bobskill and Carlson)

APPROXIMATE STAGNATION POINT SOLUTION

OBJECTIVE:

Develop an "accurate" approximate solution suitable for parametric studies.

STARTING POINT:

Supersonic velocities and continuum flow. Later extend to lower velocities and transition region.

FLOWFIELD STRUCTURE:

		Conducting		Conducting	\
					\
		Chem. Noneq.		Chem. Eq.	\
U					\
		Complete Dissoc.		Complete Dissoc	\
		in Shock Front			\
p					\
		Ambipolar Diffusion		No Mol. Diff.	\
					\
		$u \approx 0$		$u \approx \text{zero}$	\
		$p \approx \text{constant}$		$p \approx \text{constant}$	\
					\
		Radiative Losses		Radiative Losses from	\
		Dominated by VUV		Optically Thin Part of	\
				Spectrum	\
					\
		$T_H \neq T_e$		$T_H = T_e$	\
					\
		T_e Constant			\
Bow Shock				End of Noneq. Zone	Wall

GOVERNING EQUATION:

$$\begin{aligned}
 \rho u \frac{dh}{dx} + \frac{d}{dx} \left[\sum_{i=1}^s (1-\lambda_i) \frac{dT_i}{dx} \right] + \frac{d}{dx} \left[\sum_{i=1}^s \rho_i U_i h_i \right] \\
 + \frac{dq_R}{dx} - u \frac{dp}{dx} = - \sum_{i=1}^s \dot{w}_i h_i^0
 \end{aligned}$$

TWO TRANSFORMATIONS:

$$(1) \quad d\bar{n} = \bar{\rho}^{1/2} d\bar{x} \quad \Rightarrow \quad \bar{\rho} \bar{u} = -\bar{n}$$

$$(2) \quad d\tau_i = \frac{K_i L}{\bar{\rho}^{1/2}} d\bar{n}$$

Prandtl No. = constant; $\bar{\rho}^{1/2} \bar{\mu} = 1$

THICK ZONE

ABSORPTION COEFFICIENT

$$K_T = K_{T_s} \bar{\rho}^{1/2} \quad (\text{Allows } K_T \text{ to depend upon flowfield})$$

RADIATIVE TRANSFER:

$$-\frac{d \dot{q}_{R_i}(\tau_i)}{dx} = -4\pi K_i S_i + 2\pi K_i \int_0^\infty S_i E_1(\tau_i - z_i) dz_i$$

approximated as

$$-\frac{d \dot{q}_{R_T}}{dx} = -2\pi K_T S_{T_e} \exp(-2\tau_T)$$

CHEMISTRY:

"Uncouple" Chemistry by Assuming

$$P_x/\rho = \epsilon = \epsilon(\bar{n}, \tau_T)$$

for now

$$\epsilon = \epsilon_{eq} [1 - \exp(-B \tau_T)]$$

where B is expt./empirical

THICK EQUATION:

$$\frac{A}{\text{RePr}} h'' - \left(1 - \frac{\chi_T}{A}\right) h' = \Gamma_T e^{-\beta \chi_T} + \left[\left(1 - \frac{\chi_T}{A}\right) C - \frac{A}{\text{RePr}} D \right] e^{-\beta \chi_T}$$

$$A = K_{fs} L \quad \Gamma_T = \frac{2\pi S_{Ts}}{\rho_s u_s h_s} \quad C = (\bar{h}_I^0 - \bar{h}_A^0) \epsilon_{eg} \cdot B$$

$$D = \bar{h}_e \epsilon_{eg} B^2 \quad \text{Re} = \frac{\rho_s u_s h_s}{L} \quad \bar{n} = 1 - \frac{\chi_T}{A}$$

SHOCK B.C. :

Includes thermal conduction
Actual value coupled to the solution

THIN ZONE

ABSORPTION COEFFICIENT:

$$K_t = K_{t_0} \left(\bar{p} / \bar{p}_0 \right)^{1/2}$$

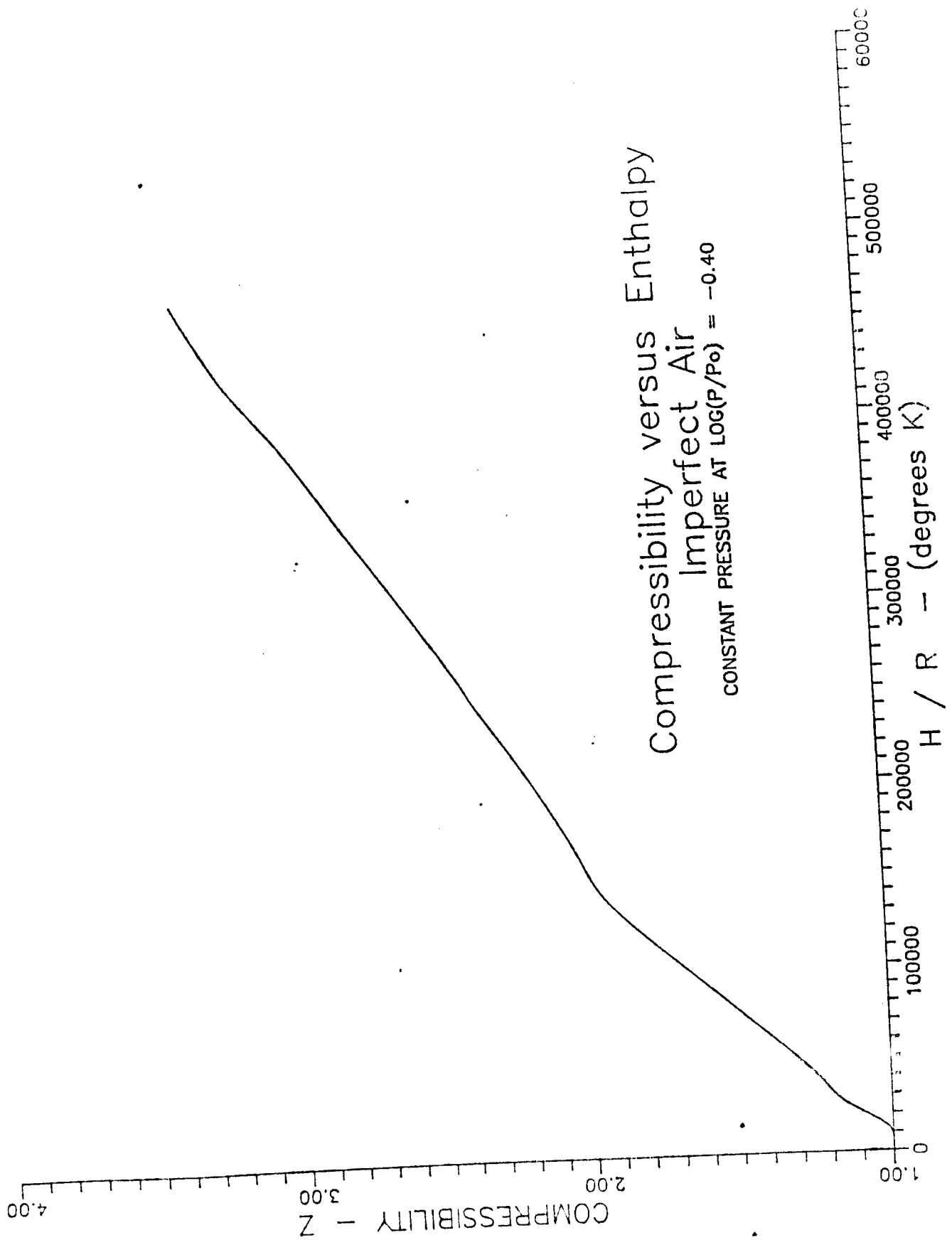
RADIATIVE TRANSFER:

$$\frac{d \dot{q}_R}{dx} = E_{t_0} \left(\frac{\rho}{\rho_0} \right)^{1/2} \left(\frac{\bar{h}}{\bar{h}_0} \right)^n$$

where n is typically 3

CHEMISTRY:

Assume $\epsilon = \epsilon(\bar{h})$ and use linear segments.



WALL B. C.:

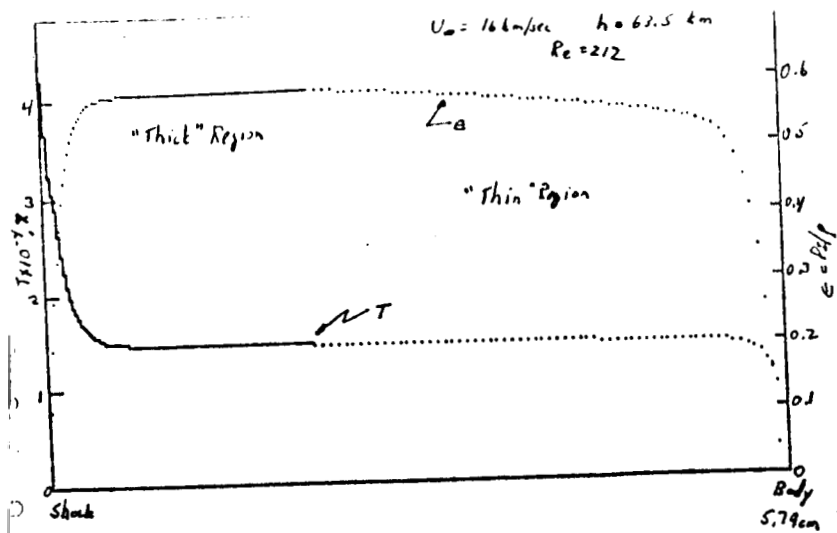
Currently assuming "hot" noncatalytic wall.

THIN EQUATION:

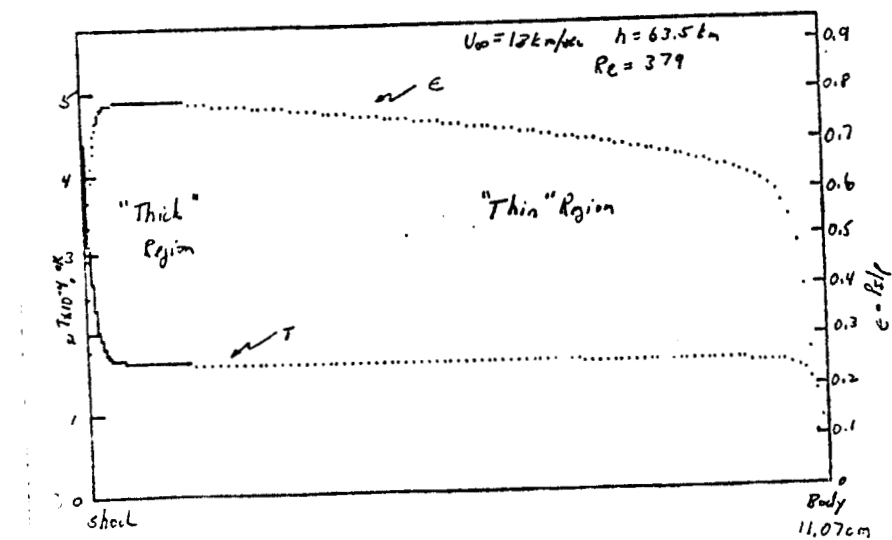
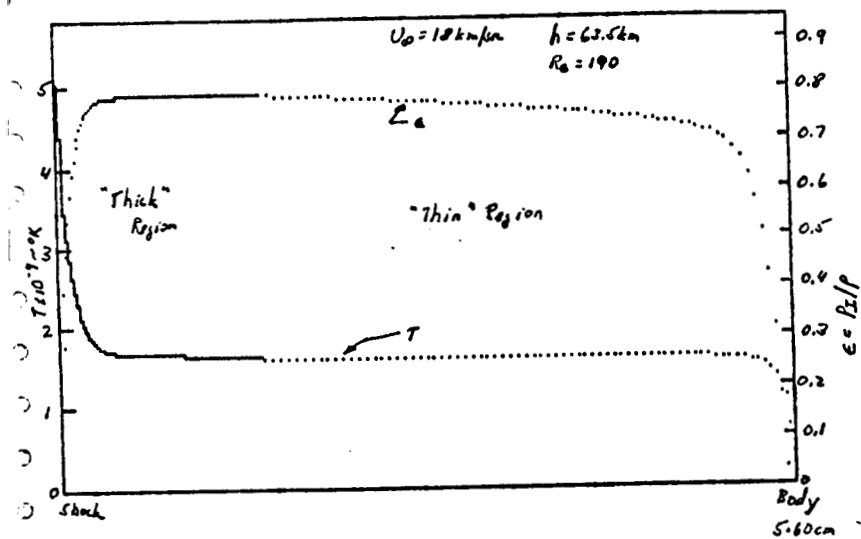
$$\left[1 - \frac{\tau_t}{\tau_{t,w}} \right] \left[1 + a \left(\bar{h}_r^o - \bar{h}_a^o \right) \right] h' - \frac{\tau_{t,w}}{\text{RePr}} h'' = - \frac{\eta_t}{K_{t_0} L} \left(\frac{\bar{h}}{\bar{h}_0} \right)^n$$

PHYSICAL COORDINATES:

Obtained from solution and transformations.



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Approx. Fire II Trajectory Point

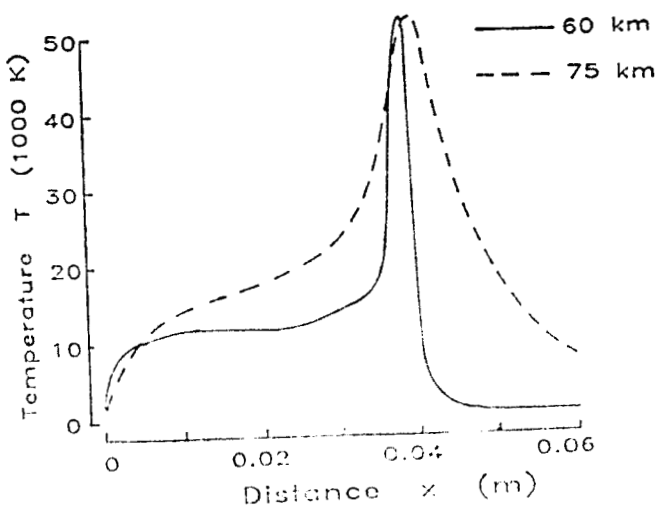
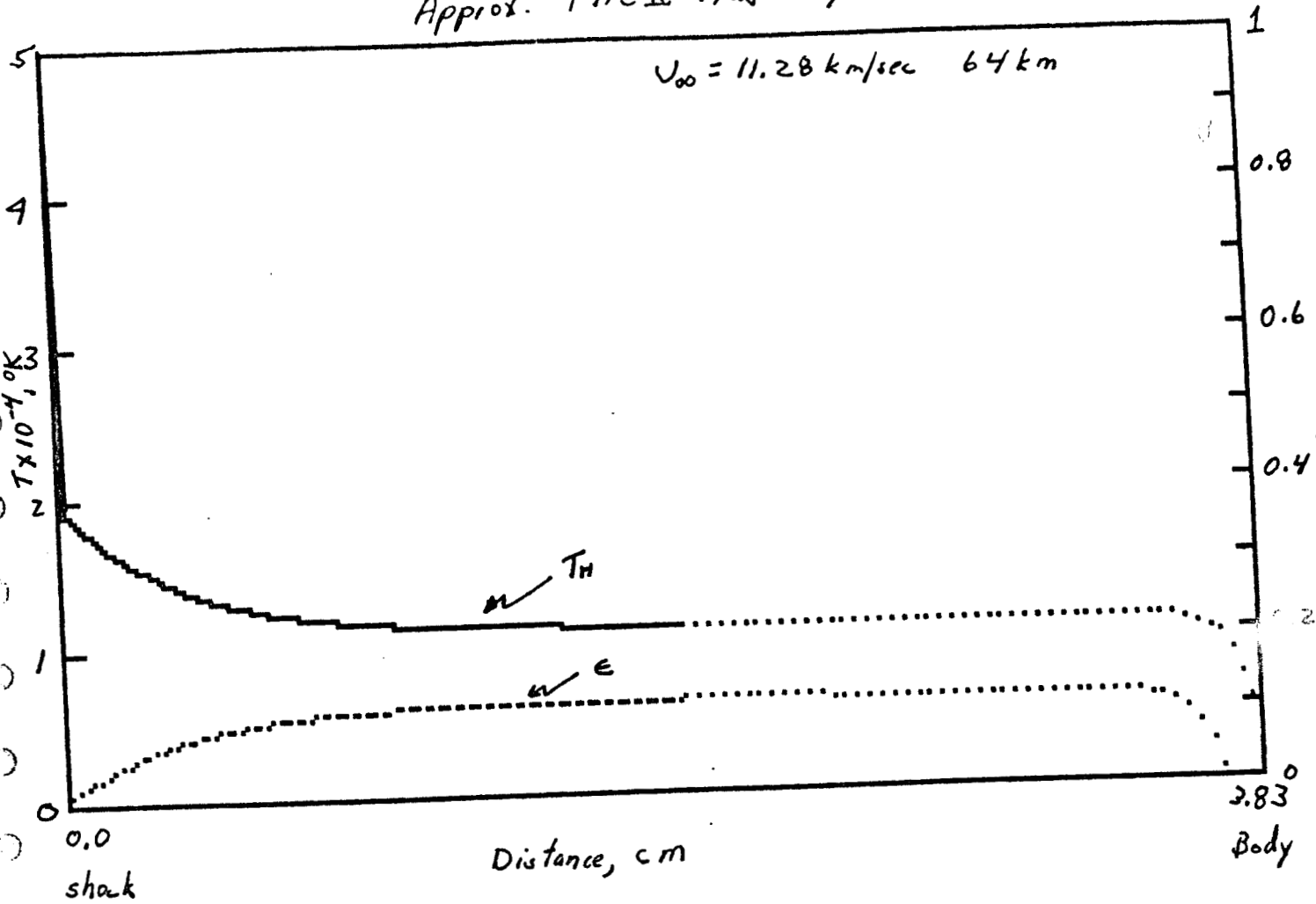


Fig. 5. The temperature profiles along the stagnation streamline.

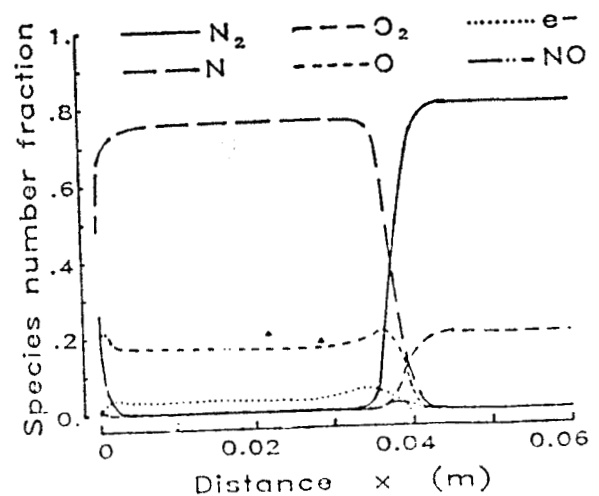
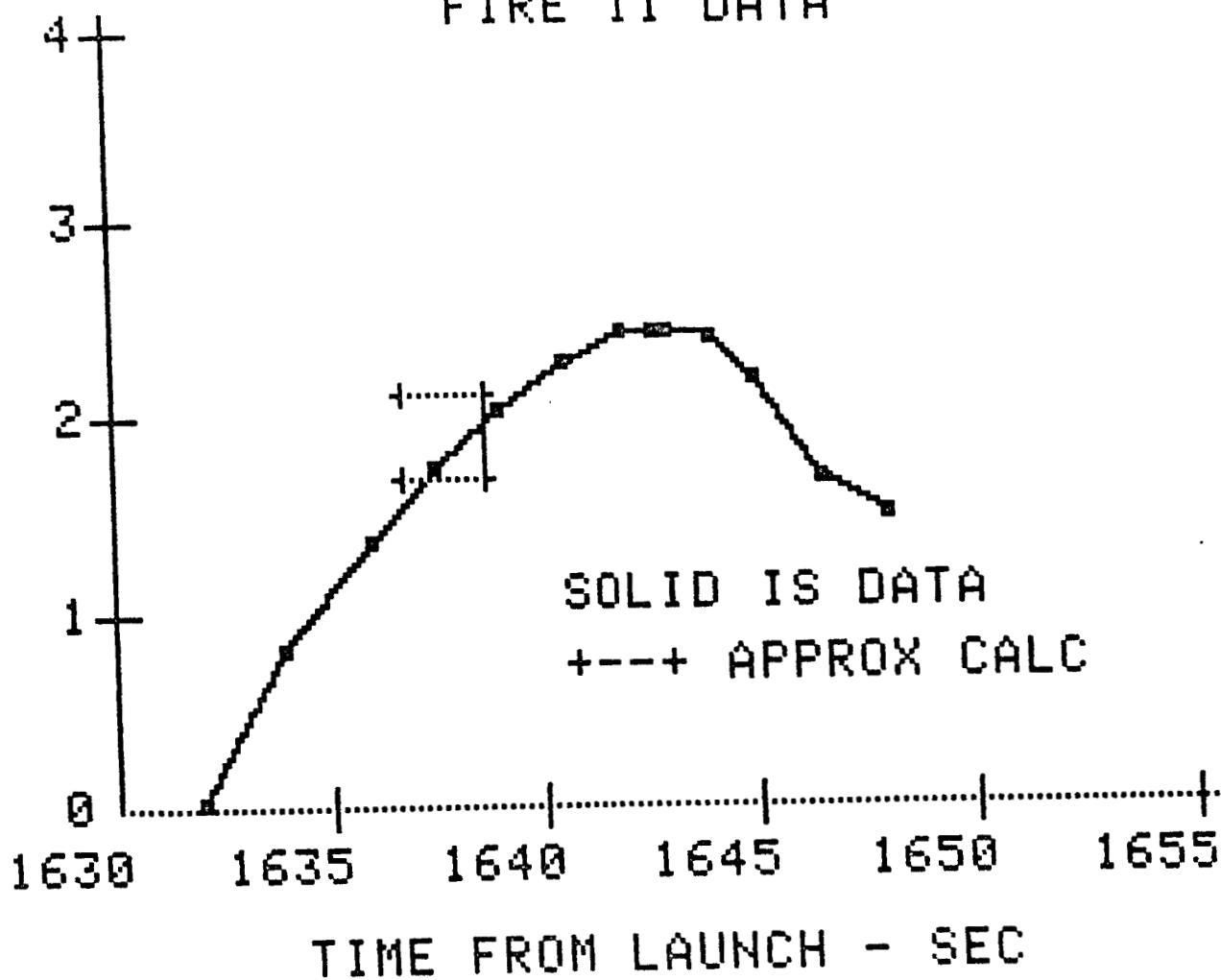


Fig. 6. Flow composition along the stagnation streamline at 60 km.

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FIRE II DATA



FUTURE EFFORTS

1. Accurately compute radiative heat transfer using a 5-step model.
2. Compute convective heat transfer.
3. Incorporate nonequilibrium effects on absorption coefficients.
4. Improve relaxation "distance" values.
5. Improve chemistry correlations.
6. Improve match points and thick downstream boundary condition.
7. Automate
8. Compare to data and perform parametric studies.
9. Extend further into AOTV/AFE flight regime.

APPROXIMATE FLOWFIELD SOLUTION STUDIES

FLOWFIELD MODEL

Using a nonequilibrium Maslen type of model due to Grose.

Advantages:

1. Fast
2. Can do individual streamlines
3. Should model AOTV/AFE reasonably well

Usage:

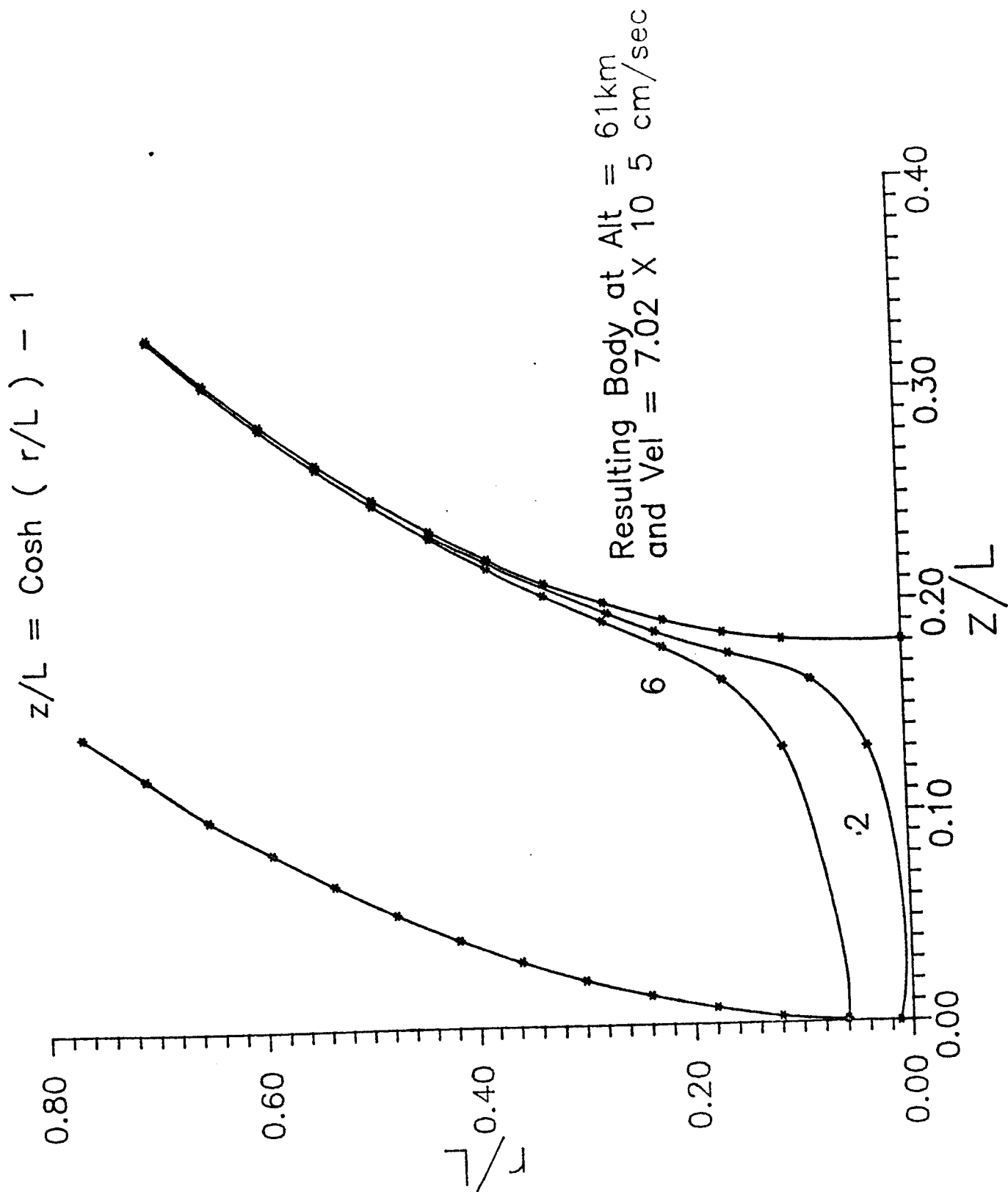
1. Study Shock, TE, and Radiation Models
2. Study Vibrational-Chemistry Temperature Coupling models
3. Study reaction chemistry models

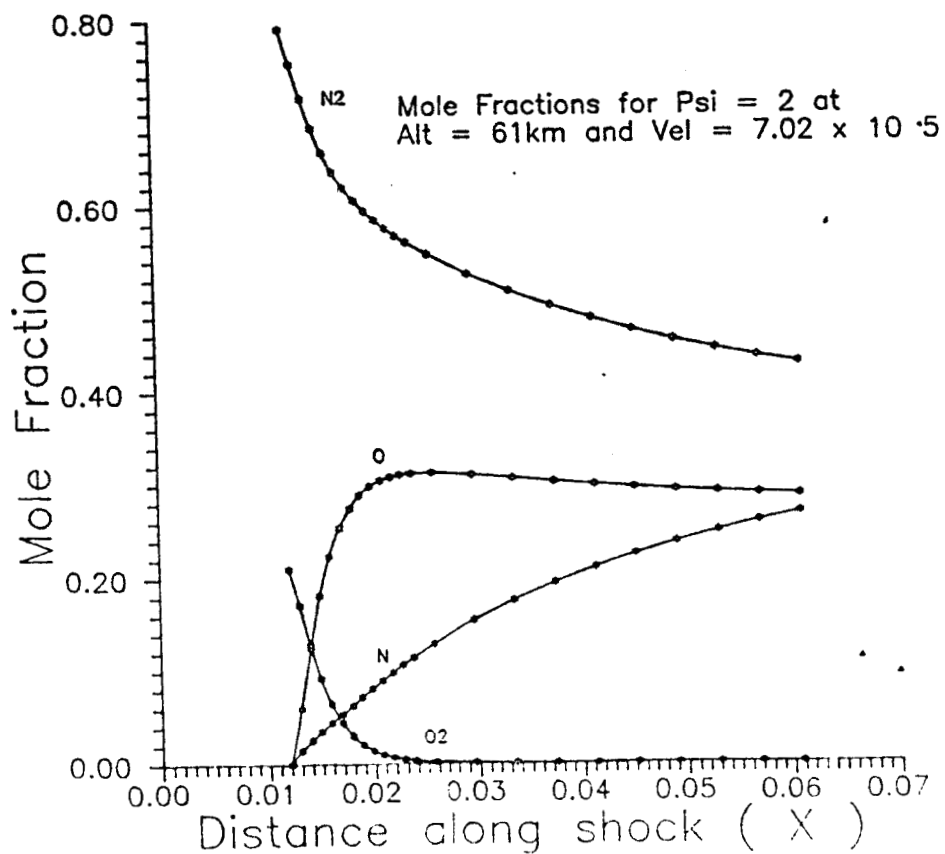
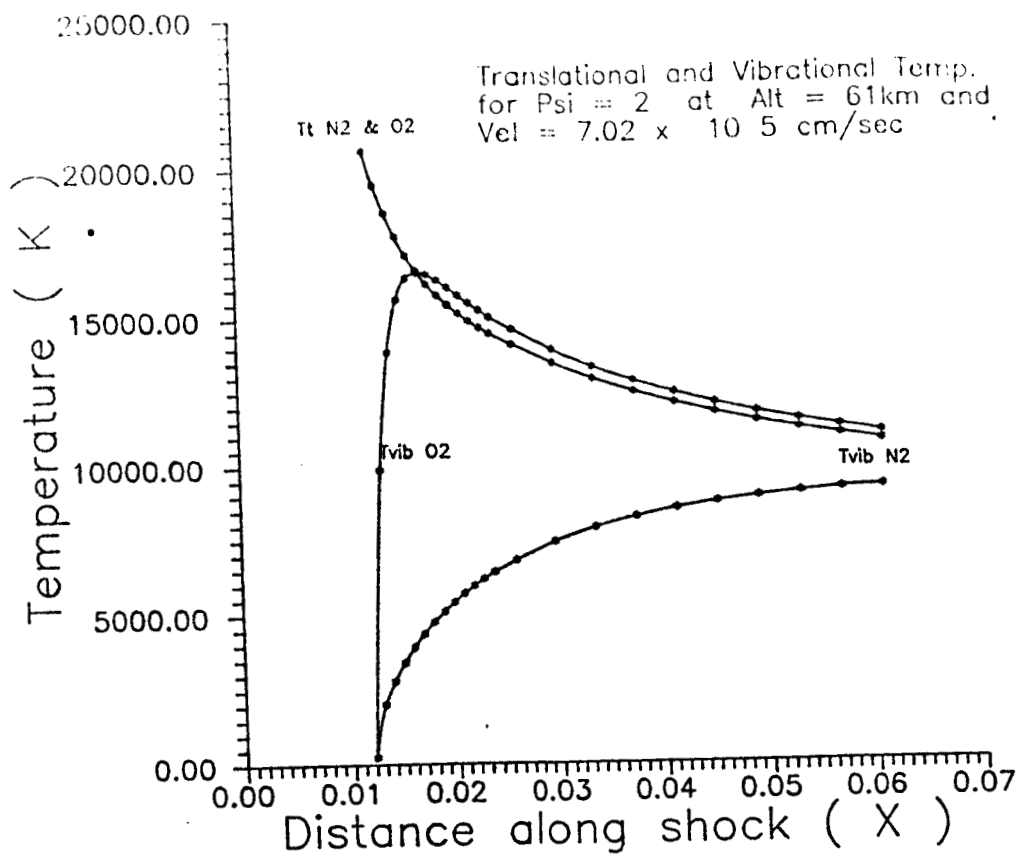
SHOCK JUMP APPROXIMATIONS

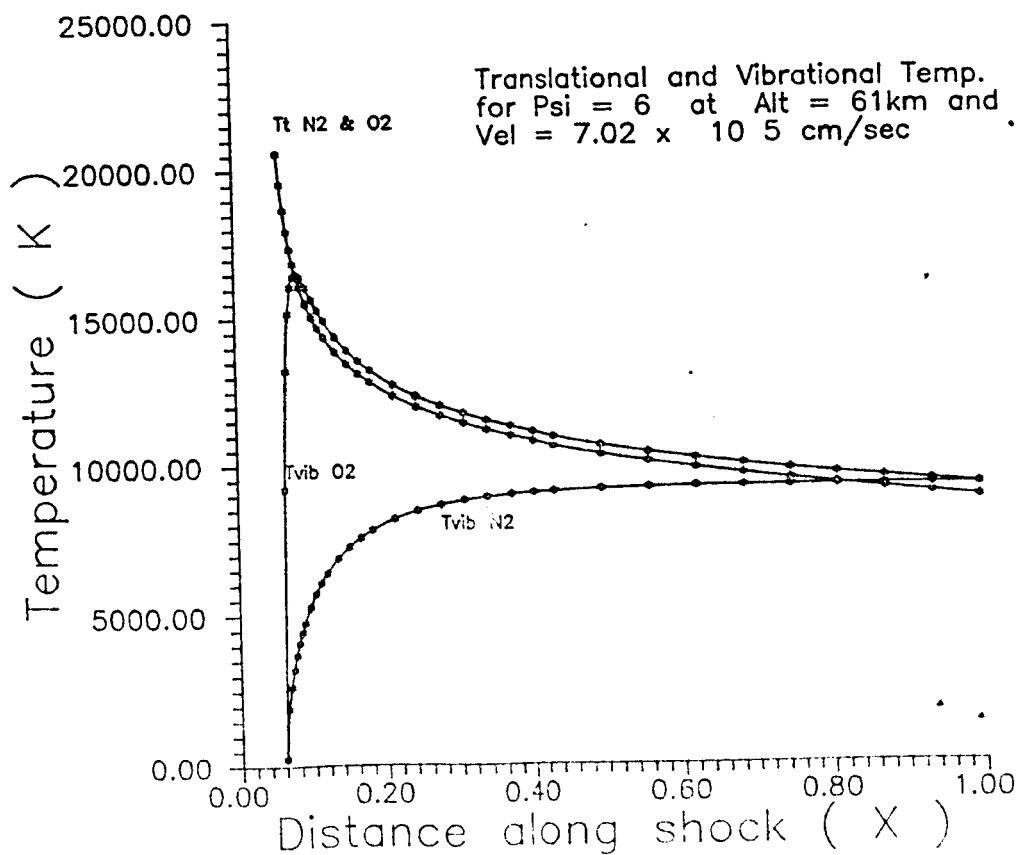
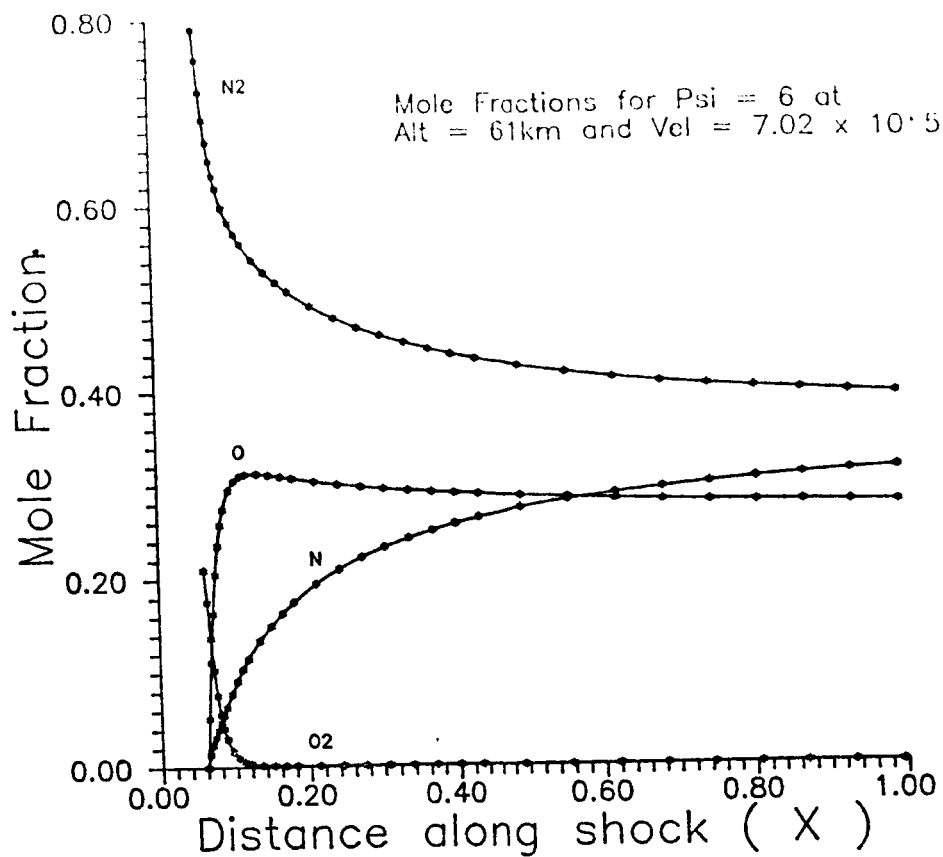
Currently developing four different cases:

- (1) Frozen
- (2) O₂ & O in equil., N₂ frozen
- (3) Pure N₂ with N₂ & N in equil.
- (4) N₂, O₂ in equil. with N & O

Plan to determine where approx. applicable, subsequent effects on flowfield, and computational effort involved (savings).







ELECTRON TEMPERATURE MODELS

At high temperatures, can TE be approximated or must a TE DEQ be solved? How can problem be simplified?

When significant number of molecules present, TE is coupled to TVN2. But how is it coupled? Is TE=TVN2 okay? Is a more detailed model needed?

Previous results --

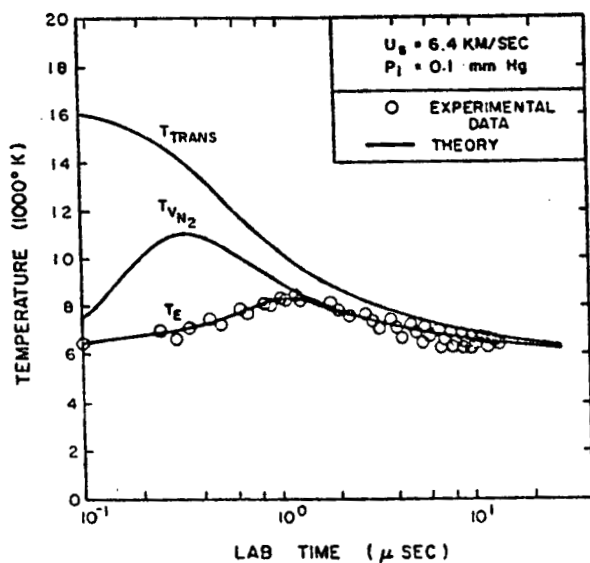


FIG. 3. Comparison of theoretical prediction and experimental data for electron temperature.

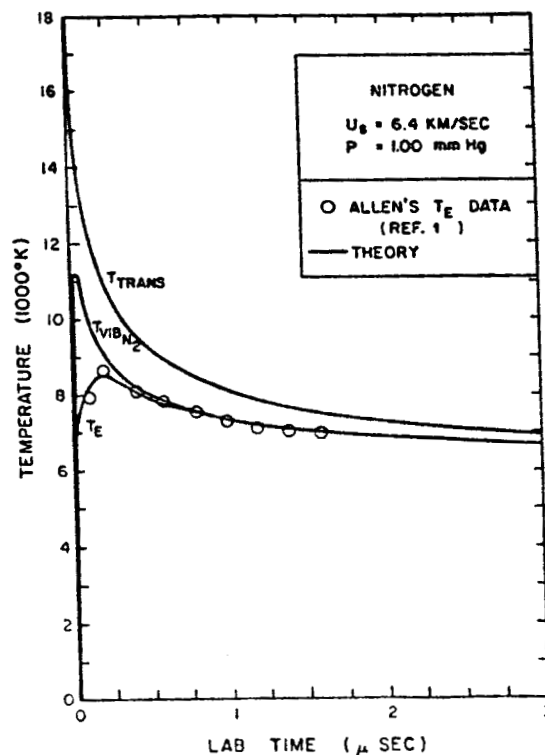


FIG. 4. Comparison of theoretical prediction based upon present experiments with experimental measurements of Allen (Ref. 1).

RADIATION MODELS

At high temperatures, above 8000 to 10000 K, flow consists of atoms and ions. Step models (5) appear adequate, but possibly can be simplified. Radiation gasdynamic coupling probably important.

When molecular radiation important, can step models be used? How many steps? Radiation coupling probably not important.

VIBRATION-CHEMISTRY COUPLING MODELS

Various possibilities exist:

1. CVDV
2. CVDV Preferential
3. Park Model

Influence of vibrational relaxation data and correlations?

The similarities, differences, and consequences of using each of these models in the AOTV regime needs to be determined.

REACTION CHEMISTRY MODELS

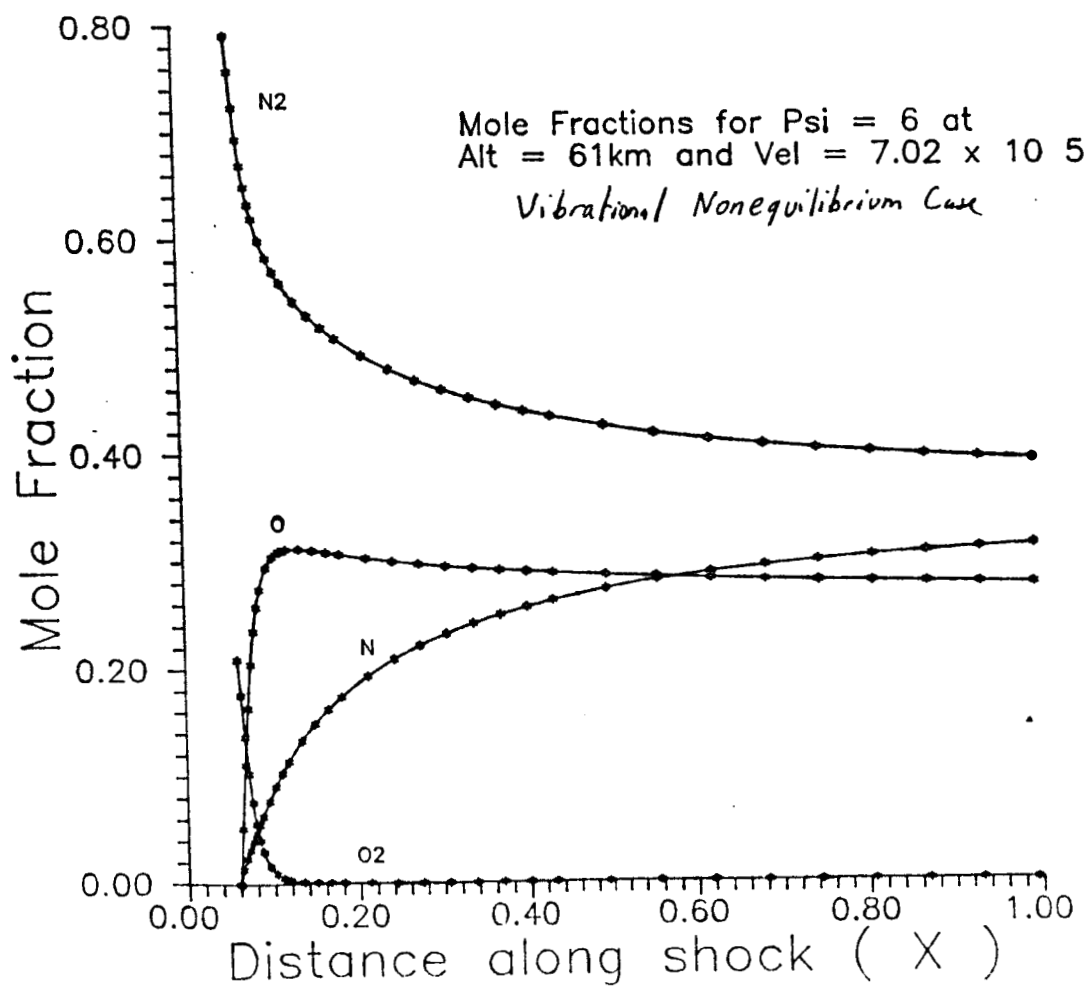
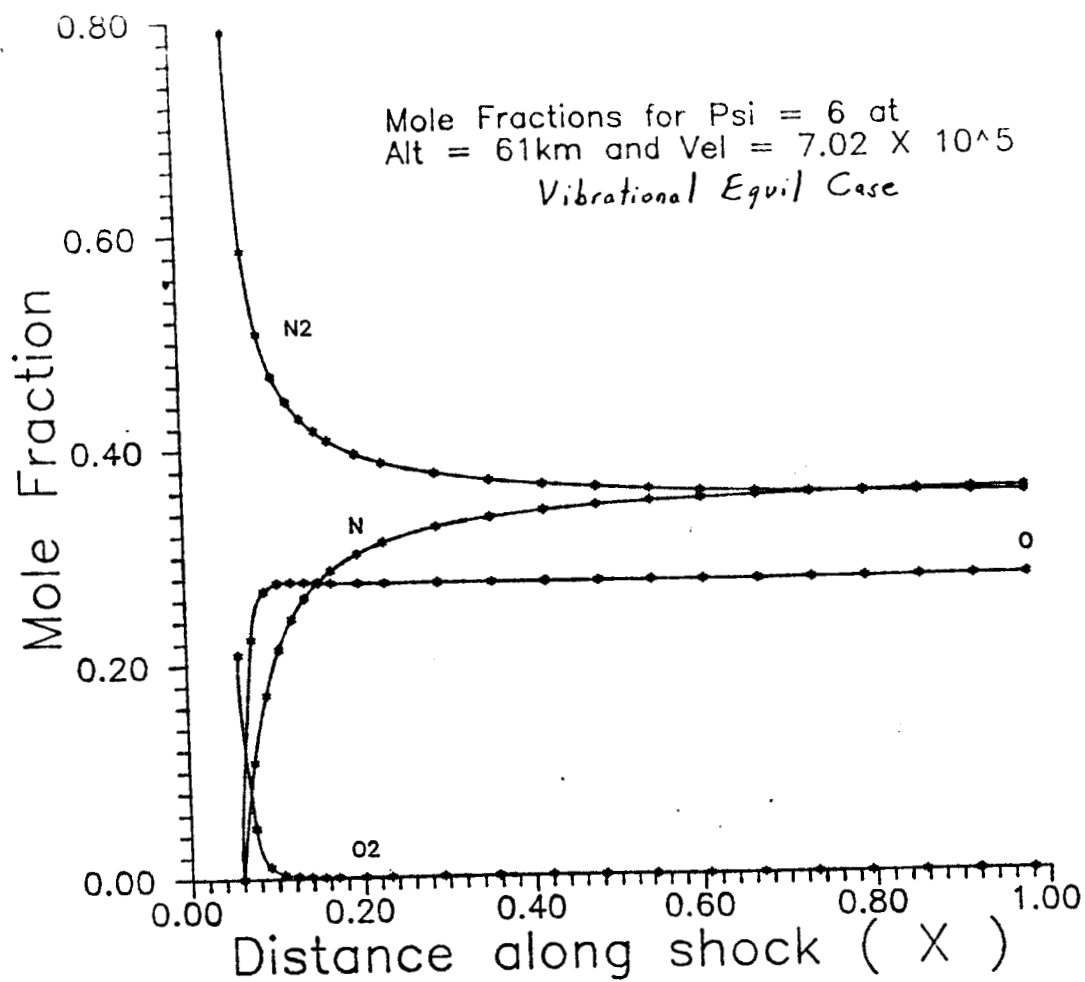
Must be studied in conjunction with vib-chem. models.

Study influence of number of species and number of reactions on flowfield structure and computational effort.

Perform parametric studies on rates.

Study effect of various proposed reaction rate temperature dependence models.

Significant information probably could be obtained by studying only two streamlines.



FUTURE DIRECTIONS

1. Parametric studies of shock jump, electron temperature, and radiation models.
2. Parametric studies of vibration chemistry coupling and reaction chemistry models.
3. Evaluation of various models.
4. Continue to develop approximate stagnation point solution.

NOTE: Are these acceptable? We want to provide results that are of value to you! Guidance Please! Duration? Renewal? etc.